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OPTIMIZATION OF STYRENE FROM ETHYLBENZENE CASE STUDY

By

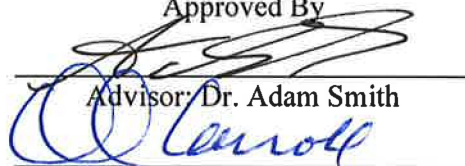
Jabria Daria Thompson

A thesis submitted to the faculty of The University of Mississippi in partial fulfillment of the requirements of the Sally McDonnell Barksdale Honors College.

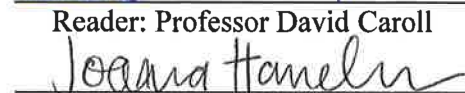
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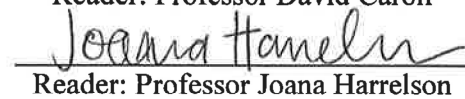
Approved By

A handwritten signature in black ink, appearing to read "Adam Smith", is written over a horizontal line.

Advisor: Dr. Adam Smith

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Reader: Professor David Carroll

A handwritten signature in black ink, appearing to read "Joana Harrelson", is written over a horizontal line.

Reader: Professor Joana Harrelson

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First, I would like to extend my gratitude to my teammates, Beck Fletcher and Carly Huguley. Not only did they contribute to the completion of this thesis through their persistent work ethic, but they contributed to my personal life as well through their genuine care and support. I am greatly appreciative of both and could not imagine a better group with whom I would want to end my college career.

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ABSTRACT

JABRIA DARIA THOMPSON: Optimization of Styrene from Ethylbenzene Case Study

(Under the direction of Dr. Adam Smith)

The following pages detail the optimization process of styrene from ethylbenzene in the Styrene Production Plant, Unit 500. There were two parts of the assignment, each with slightly different end goals. The goal of the first part of the assignment, was to create a process that would effectively and efficiently increase the negative Net Present Value (NPV) of the production plant. Procedures taken in this process included developing a working kinetic process simulation model and optimizing this model through unit operations and heat integration, as well as developing an accurate economic model that will be used to evaluate the proposed process and support optimization alternatives. Through optimization, the NPV for the base case increased by \$375M from a starting value of (\$920M). The findings determined that with further optimization of the process, the net present value of the plant has the potential to increase tremendously. The second part of the assignment focused on the optimization of an isothermal fluidized bed reactor using the same reactions and kinetics in part 1. Similar procedures and calculations were taken to simulate the process, but with the main objective function being the selectivity of styrene. Through optimization, a high selectivity was able to be obtained, however, it was determined that other aspects of the process suffer as a result. Thus, it is able to be concluded that what may be initially perceived as an “optimum value” is not always beneficial to the process.

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LIST OF SYMBOLS

u_{mf}	minimum fluidizing velocity
d_p	particle diameter
ρ_g	gas density
ρ_s	catalyst density
μ_g	gas viscosity
g	acceleration of gravity

PART 1: STYRENE CASE STUDY

Introduction

The goal of the project was to optimize a proposed styrene production process designed to operate 8,000 hours (about 11 months) per year and produce 100,000 metric tonnes per year of 99.8% by weight styrene via the dehydrogenation of ethylbenzene. A Process Flow Diagram (PFD), which can be found in Appendix A, was given as a starting design along with initial process parameters and conditions. An excel model designing the required numerical values at each stage was completed and used to determine the economics of the project. The project was modeled using PRO/II software and an excel model was used to determine the economics of the project. PRO/II was then used to optimize the project through changing equipment layout, design specifications, and change process conditions to reduce the cost of building the plant.

Base Case

The base case ethylbenzene feed stream is 98% by mole ethylbenzene, 1% benzene, and 1% toluene and enters at 136°C and 210 kPa. The thermodynamic package used was SRK-SIMSCI because of the presence of aromatic compounds. This feed stream then mixes with an ethylbenzene recycle stream before being heated by heat exchanger E-501 with condensing high-pressure steam as its utility. This stream then mixes with superheated steam to increase the temperature of the process stream to 550°C before entering the endothermic reactor series. The packed bed adiabatic reactor was set with the following reaction system:

$$C_6H_5C_2H_5 \rightleftharpoons C_6H_5C_2H_3 + H_2 \quad r_1 = 6.2 \exp\left(\frac{-90,981}{RT}\right) p_{eb} \quad (\text{forward})$$

$$r_2 = 6 \times 10^{-5} \exp\left(\frac{-61,127}{RT}\right) p_{sty} p_{H_2} \quad (\text{reverse})$$

The following side reactions also take place:

$$C_6H_5C_2H_5 \rightarrow C_6H_6 + C_2H_4 \quad r_3 = 2.71 \times 10^7 \exp\left(\frac{-207,989}{RT}\right) p_{eb}$$

$$C_6H_5C_2H_5 + H_2 \rightarrow C_6H_5CH_3 + CH_4 \quad r_4 = 6.45 \times 10^{-4} \exp\left(\frac{-91,515}{RT}\right) p_{eb} p_{H_2}$$

Where p_i is the partial pressure of component i in Pa, T is the temperature in K, the activation energy is in J/mol, and the rate is in mol/(m³ catalyst*second). R-501a-e was modeled as a single packed bed reactor with five tubes.

The reactor effluent from R-501a-e was then sent to E-502 where it was heated to 575°C using the remainder of the superheated steam generated by H-501. The process stream then enters the second reactor series R-502a-e, which was modeled as an adiabatic packed bed reactor with five tubes.

The superheated steam is generated by heating low pressure steam to 800°C using a steam heater, H-501. The superheated steam then splits, with part going to heat the ethylbenzene stream and the rest going to the utility side of exchanger E-502.

The reactor effluent is then cooled by three heat exchangers in series. The first heat exchanger, E-503 uses condensing high pressure stream to cool the process stream to 270°C. The

stream is then cooled to 180°C by E-504 which utilizes condensing low-pressure steam. Finally, cooling water in E-505 cools the stream to 65°C. At this temperature some of the stream will have condensed and the two liquid phase SRK-SIMSCI package should be used to distinguish between the aqueous and organic liquid phases.

The process stream enters a three-phase separator, V-501. The vapor phase leaves from the top of vessel where a valve is then used to adjust the pressure. The liquid water phase leaves from the bottom of V-501 where the pressure is then increased in P-501 before leaving the process as wastewater.

The liquid organic phase leaves from the middle of the vessel and is sent to a Benzene/Toluene Column, T-501. This column has a total reboiler and a partial condenser. The tower specifications were set so that 99% of the toluene was recovered in the distillate, 99% of the ethylbenzene was recovered in the bottoms, and the condenser temperature was 50°C. The vapor component of the distillate leaves the reflux drum from the top and mixes with the vapor component of the three-phase separator. This stream is then compressed in C-501 before leaving the process as fuel gas. The liquid component of the distillate is pressurized in pump P-504 and then leaves the process as a benzene/toluene product stream.

The bottoms of T-501 require further separation and are sent to a styrene column, T-502 to purify the styrene product. This column has a total condenser and reboiler. The tower specifications were that 99% of the styrene should be recovered in the bottoms at a purity of 99.8% by weight. The distillate stream, or ethylbenzene recycle, is pressurized in P-506 before mixing with the ethylbenzene feed stream. The bottoms of T-502 are pressurized in P-505 before leaving the process as the styrene production stream. A controller was used to calculate the

flowrate of the ethylbenzene feed stream required to produce 100,000 metric tonnes per year of 99.8% by weight styrene.

Economics

The economics were determined through updating a model created in excel that determines all costs associated with the startup and production of the styrene process. Using a stream table generated in PRO/II, the required raw materials were determined to be 25,300 kg/h of ethylbenzene, 146,800 kg/h of low-pressure steam (lps), and a 25,600 kg/h ethylbenzene recycle to produce the required 12,500 kg/h (100,000 tonnes/yr) of styrene. The equipment was sized to fit these needs according to the previously designed PFD provided to the team for the exploration of the styrene process. The material of construction (MOC) components of all machinery needed were given and used when factoring in the equipment cost. The total costs for the equipment are: \$11.6 million for the heat exchangers, \$140,000 for required pumps/drives, \$21.7 million for a heater, \$7.1 million for the two reactors, \$400,000 for the required vessels, \$17.9 million for a compressor, \$5.8 million for tower T-501, and finally \$80 million for tower T-502 which totals to about \$205 million. Along with the equipment cost, materials have a cost of \$225 million a year, labor has a cost of \$1.5 million a year, and utility cost is \$15 million per year. All of these costs total to have a net present value (NPV) of about \$920 million dollars and an annual equivalent cost (AE) of \$150 million per year.

It can be seen in the **Error! Reference source not found.** that the two biggest cost factors are raw materials and the price of styrene. These costs are unavoidable due to the need for raw materials to produce styrene and the price of styrene being set by the current market. The amount of raw materials can be reduced, which in turn reduces operational cost, through optimization of the styrene process, but it is a cost that will remain in the NPV. However, there are other areas of

interest displayed on the sensitivity graph that are not the cost scale of raw materials and styrene, but still offer areas to reduce cost. The operating labor and utilities used for this process offer areas of further optimization that can be conducted to continue to reduce the capital needed for

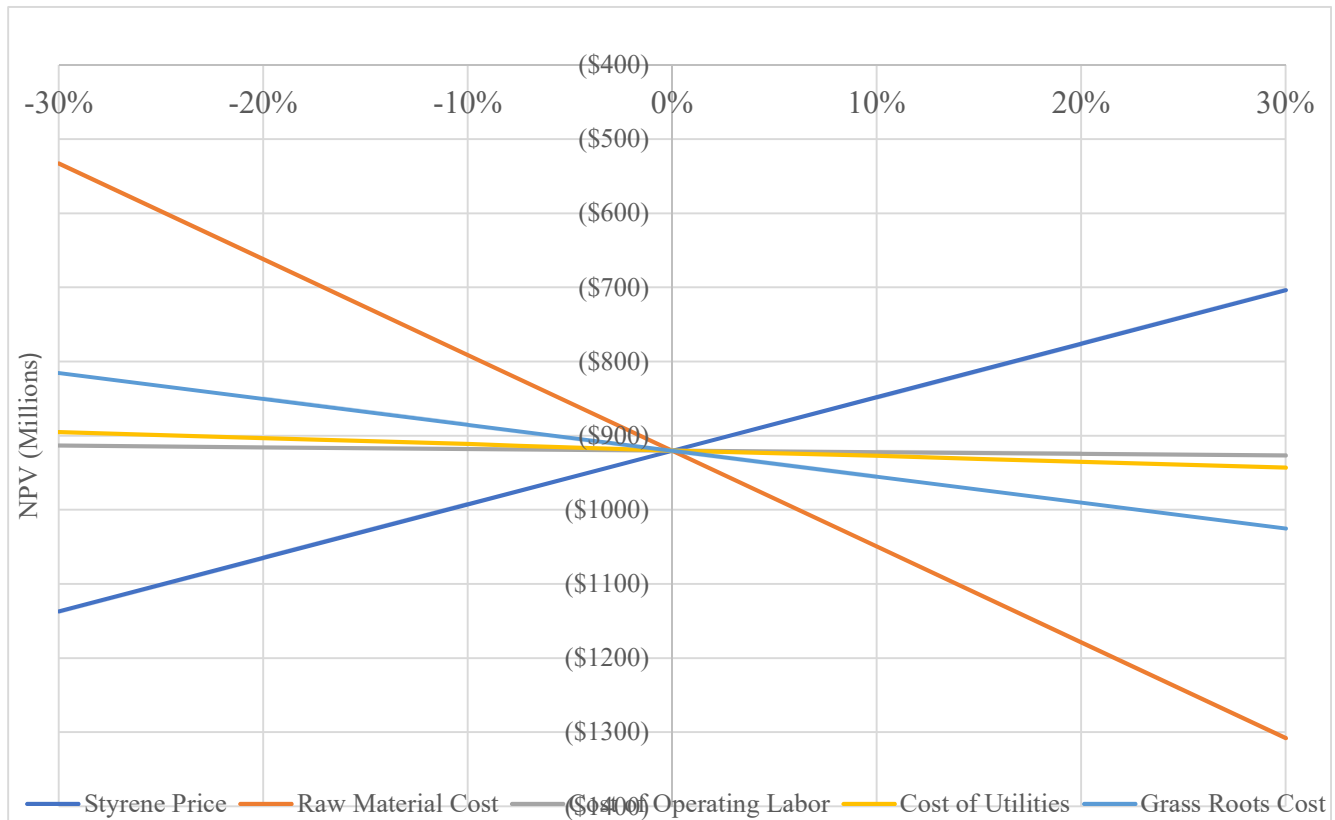


Figure 1: Base Case Sensitivity Chart

the NPV.

Current Issues

The base case NPV does not accurately reflect the final cost of the project to produce 100,000 tonnes of styrene per year. There are many areas for optimization that will drastically reduce the price of this project. The reactors, 3-Phase vessel, towers, utilities, and overall process conditions can be manipulated to move NPV towards the cost of purchasing the required styrene. The main cost saving areas are the equipment portion, process efficiency (more conversion of

styrene requires less raw materials), and then other things such as heat integration or the restructuring of the process layout.

In the reactor unit: inlet pressure, inlet temperature, inlet concentration, volume, pressure drop, and length to diameter ratio can all be manipulated to reduce cost. With a more efficient conversion of the raw materials, the amount of materials needed can be reduced because more styrene is being produced.

In the vessel and towers the operating conditions play a key role in determining the optimum conditions to separate the styrene out from the other components. The vessel and tower components also play a key role in conjunction with the operation conditions. Based on the vessels and towers specifications, an optimum between the trays, volumes, pressures, and temperatures will need to be considered to recover styrene most effectively.

Continuing the Project

While it may not be possible to get a number at or below the cost of purchasing styrene yearly, the added safety and isolation from market swings or supply chain issues make further exploration viable. Through optimization the project will become more realistic and make economic sense once every aspect of the project is at the most cost-effective point. By conducting optimization of the project and further exploration of the different possibilities regarding process operation the NPV will become viable.

Optimization

After completing the base case as described above, the team worked to optimize the case study. Optimization was conducted by unit operation optimization and heat integration. The unit operations were optimized in the order they appear in the Unit 500 process. After conducting unit

operation optimization, heat integration was conducted. Unit operation optimization began with the reactors, then the three-phase separatory vessel, and ended with the distillation tower section of the process.

Reactors

When optimizing the reactors section of the process, the main goal is to balance the effective use of raw material and the size of downstream equipment. As more of the ethylbenzene is converted to the desired product, styrene, the larger the recycle stream necessary to meet production rate. This increase in the recycle also increases the size of downstream equipment which causes the price of the equipment to increase. At some point, the more efficient use of raw material is outweighed by the increase in equipment cost.

The first variable considered was the inlet temperature to the first set of reactors, five reactors in parallel. The inlet temperature was increased by increasing the temperature of the superheated steam that is mixed with the ethylbenzene stream fed to the reactor. The base case inlet temperature was 523.6°C and the optimum temperature was found to be 550°C. The values considered are shown in **Error! Reference source not found..**

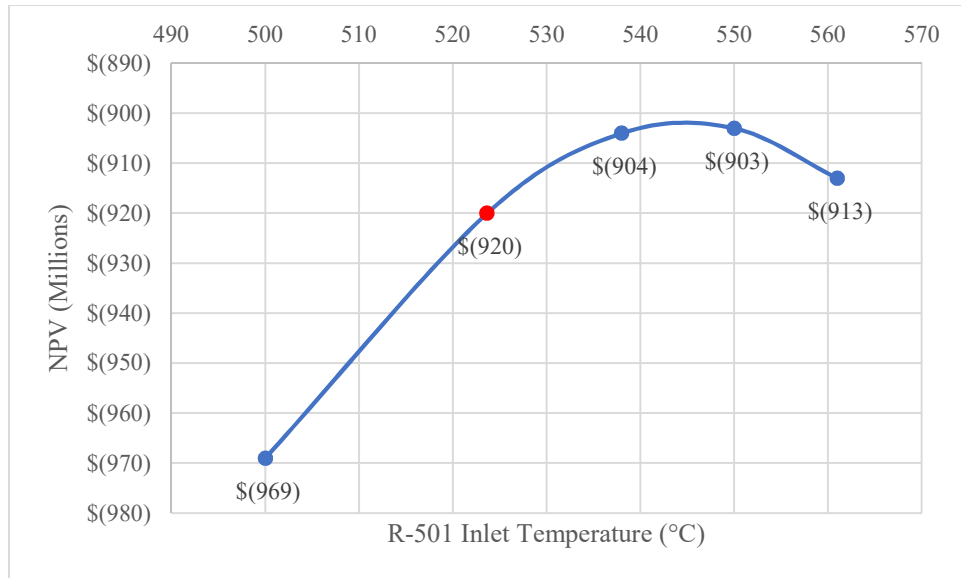


Figure 2: R-501 Inlet Temperature vs. Net Present Value

The next variable considered was the flowrate of steam dilution added to the ethylbenzene stream fed to the reactor. The amount of steam dilution changes the concentration in the reactor which in turn affects the rate of reaction. The optimum amount of steam dilution was found to be the same as the base case, 3,900 kmol/h.

Next, the inlet pressure to the first set of reactors was optimized. The inlet pressure affects the partial pressure of the components which affects the rate laws of the various reactions. The optimum pressure was found to be 235 kPa as shown in **Error! Reference source not found..** The red marker indicates the base case value.

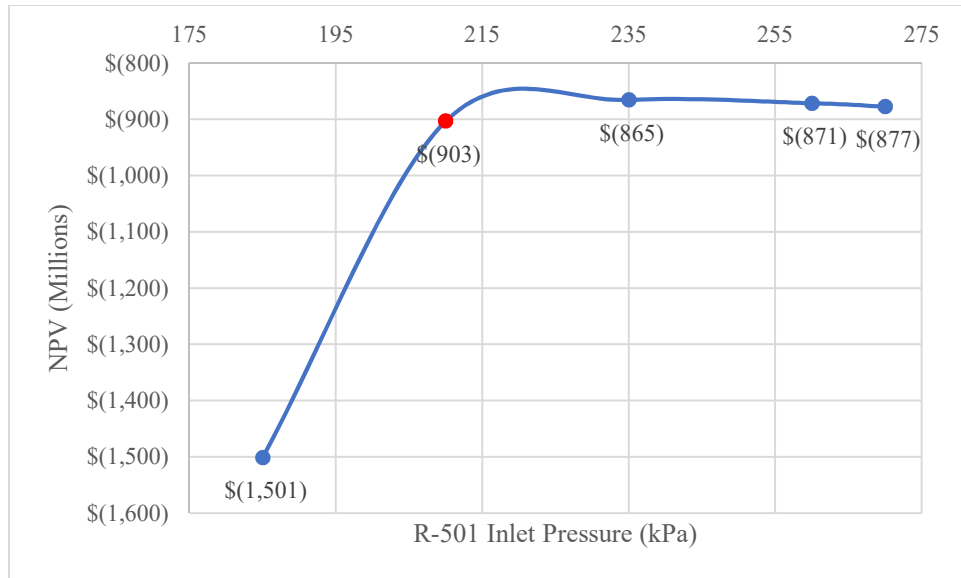


Figure 3: R-501 Inlet Pressure vs. Net Present Value

The volume of the reactors was considered next. When considering volume, both sets of reactors were changed at once. This is advantageous because if a reactor tube needs to be replaced, there is no confusion on what size tube should be used. This also means only one spare tube is needed at the plant versus two tubes of different sizes. The disadvantage of keeping the tubes the same size is the loss of ability to use the second set of reactors' volume to optimize the process. When optimizing volume, the length of the reactor varied and it was found that a volume of 55.4 m³ was the optimum value.

The length to diameter ratio (L/D ratio) of the reactors was next optimized. The L/D ratio of the optimized volume was 2. After analyzing various L/D ratios, 2 was found to be the optimum. In **Error! Reference source not found.** below, one can see that no L/D ratio less than 2 was considered. This is due to management direction that the L/D ratio should be kept between 2 to 10.

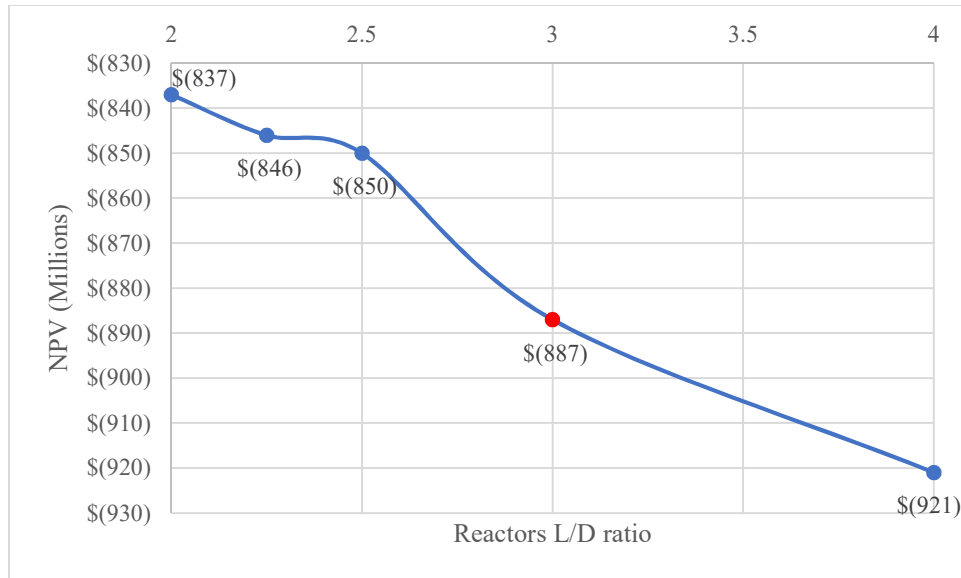


Figure 4: Reactors L/D ratio vs. Net Present Value

The final variable considered in the reactors section of the process was the inlet temperature to the second set of reactors. This set of reactors is also made up of five tubes in parallel. This temperature was adjusted by adjusting the flowrate of the superheated steam to the heat exchanger between the sets of reactors. The optimum inlet temperature to the second set of reactors was found to be 562°C from a base case value of 575°C. The net present values associated with these values can be seen in **Error! Reference source not found..**

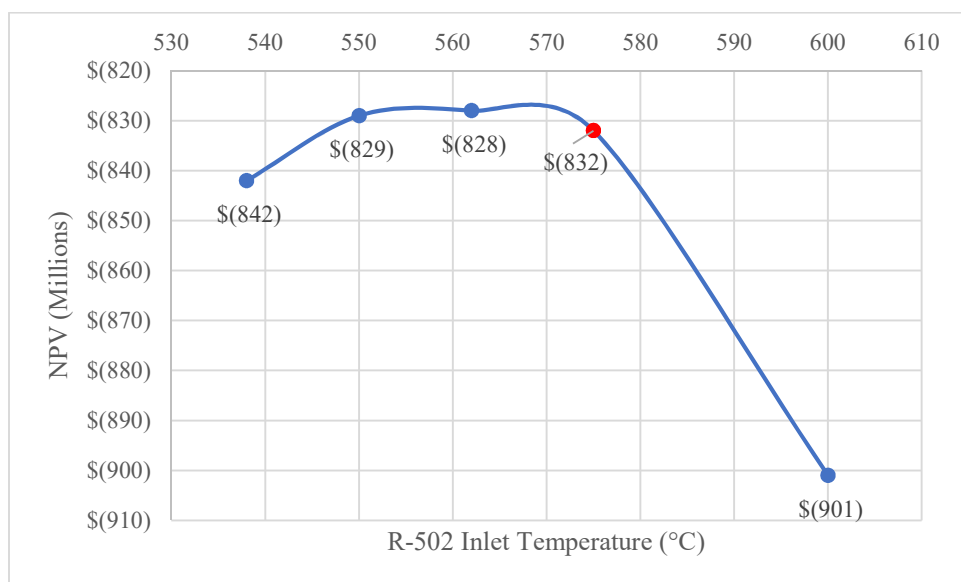


Figure 5: R-502 Inlet Temperature vs. Net Present Value

Three-Phase Separatory Vessel

In the three-phase separatory vessel, the goal is to separate the waste water and gases produced through the reactions from the organic liquid. The operating conditions of the vessel should be set so that most ethylbenzene and styrene are recovered in the organic liquid phase. This would provide the most optimum use of raw material as well as recovery of product.

When optimizing the vessel, the inlet temperature to the vessel was the primary variable considered. Using the heat exchangers and utilities present in the base case, the coldest the inlet temperature can be is 40°C. This minimum process stream temperature is due to the 10°C approach temperature set by management. This change increased the net present value by about \$90 million, but raw materials and products were still being lost to the fuel gas stream. A fourth heat exchanger was added before the three-phase separatory vessel with a refrigerated water utility (E-510). An updated three-phase separatory section of PFD is shown in **Error! Reference source not found.**

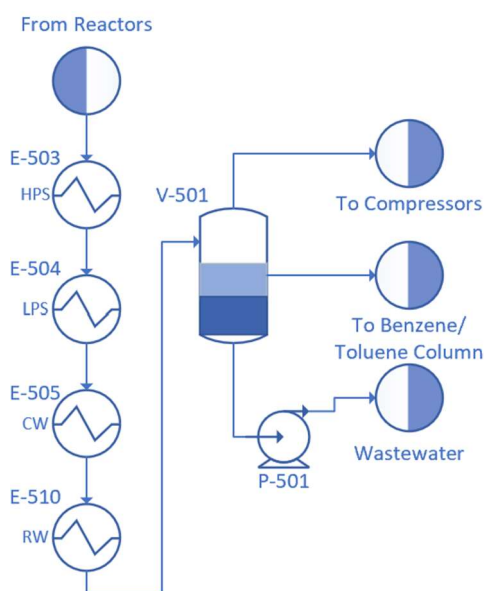


Figure 6: Separatory Vessel PFD

This added heat exchanger allowed for the process stream to be cooled to 15°C. This was found to be the optimum temperature entering the three-phase separatory vessel. To cool the process stream further, refrigerant and a fifth heat exchanger would be necessary. This was found to be less economically feasible due to the exceedingly small amount of ethylbenzene and styrene being lost to the fuel gas at 15°C. The inlet temperatures considered and their associated net present values are shown in **Error! Reference source not found..**

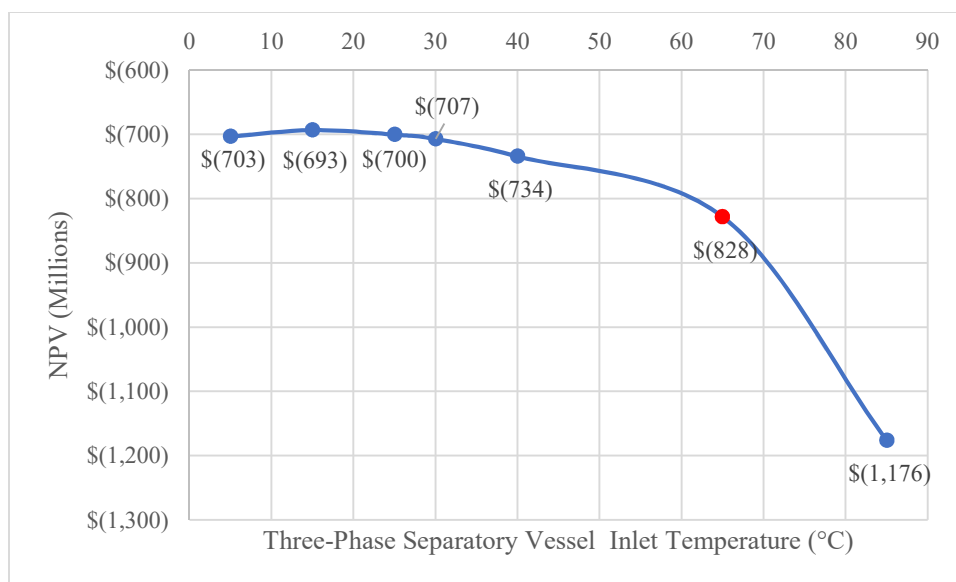


Figure 7: Separatory Vessel Inlet Temperature vs. Net Present Value

Towers

The distillation towers section of the process optimization focuses on balancing the cost of the equipment with the tower separation efficiency. The larger the tower, the easier the separation becomes but the more expensive the tower is. The smaller the tower, the greater the reflux necessary to complete the separation which causes equipment cost increase for the distillation drum and an increase in utility cost of the condenser.

First, the material of construction of the distillation tower T-501 was considered. In the base case, T-501 was constructed with titanium, however after further research using the AIChE

Chemical Reactivity Worksheet it was found that stainless steel clad would be an acceptable material of construction for all components found in the process. This change of material gave a saving of about \$10 million and a new net present value of (\$683) million.

Next the number of trays in T-501 was considered. The base case had 22 trays; however, the optimized number of trays were found to be 34. Although this causes an increase in equipment cost, the reflux decreases causing savings on utilities that outweighed the equipment cost. The number of trays considered can be seen in **Error! Reference source not found.**
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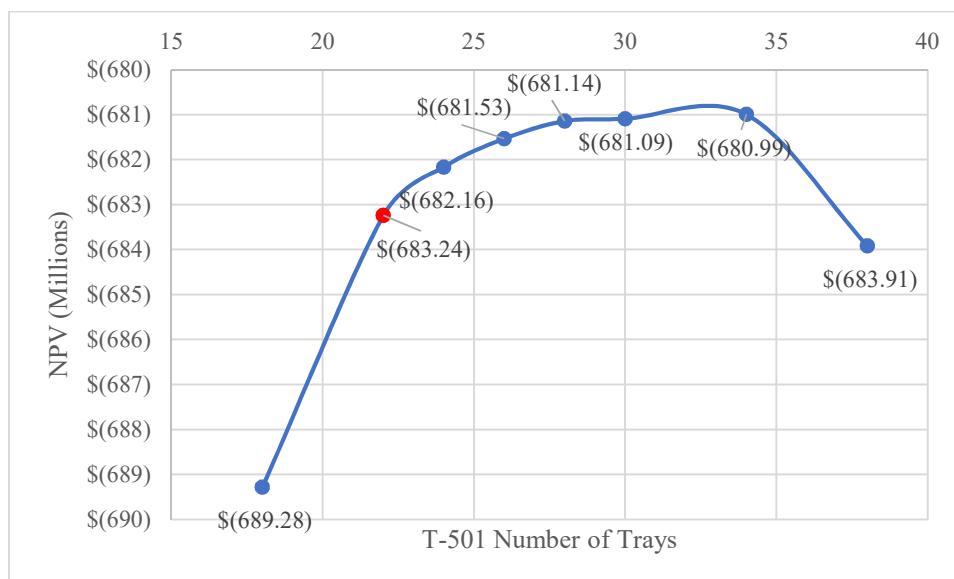


Figure 8: T-501 Number of Trays vs. Net Present Value

The top tray pressure was next optimized. While optimizing, it was found that as the top tray pressure increases, the net present value continually becomes less negative. This continual increase in net present value is due to savings in the compressor utility due to the decrease in compression ratio. Due to team concerns about the styrene column feed being greater than 125°C, at which high concentrations of styrene can spontaneously polymerize, the team chose an

optimum top tray pressure of 50 kPa. This kept the styrene column feed below 125°C and gave a final net present value of (\$678) million.

Finally, the feed tray location of T-501 was optimized. It is most optimum for the feed to the tower to enter on a tray of similar vapor/liquid fraction to the stream. If the tray enters on a tray with different vapor/liquid fractions, the efficiency of separation on that tray is depreciated.

The new feed tray location was found to be tray 16 and the trays considered can be seen in

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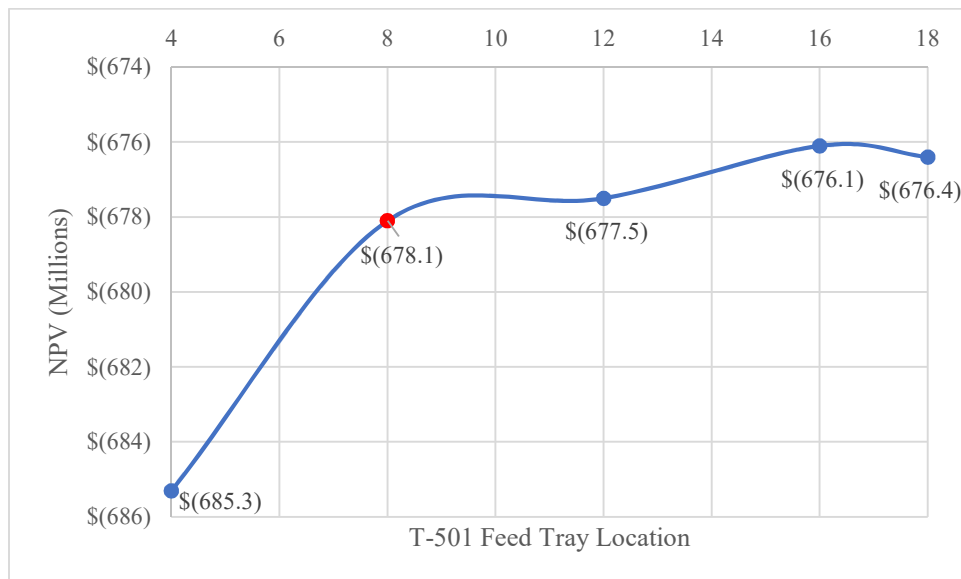


Figure 9: T-501 Feed Tray Location vs. Net Present Value

For the styrene tower, T-502, the same variables were considered. First the material of construction was changed from titanium to stainless steel clad. This provided savings of about \$120 million and increased the net present value of the project to (\$550) million.

The number of trays of T-502 was considered next. The optimum number of trays in T-502 was found to be 65 from the base case of 70 trays. The number of trays decreased due to the cost of the trays. The diameter of this tower is much bigger than the diameter of T-501, so the trays are more expensive and it is more economically feasible to increase utility cost to reach the

desired separation. The number of trays considered in the optimization process are shown in

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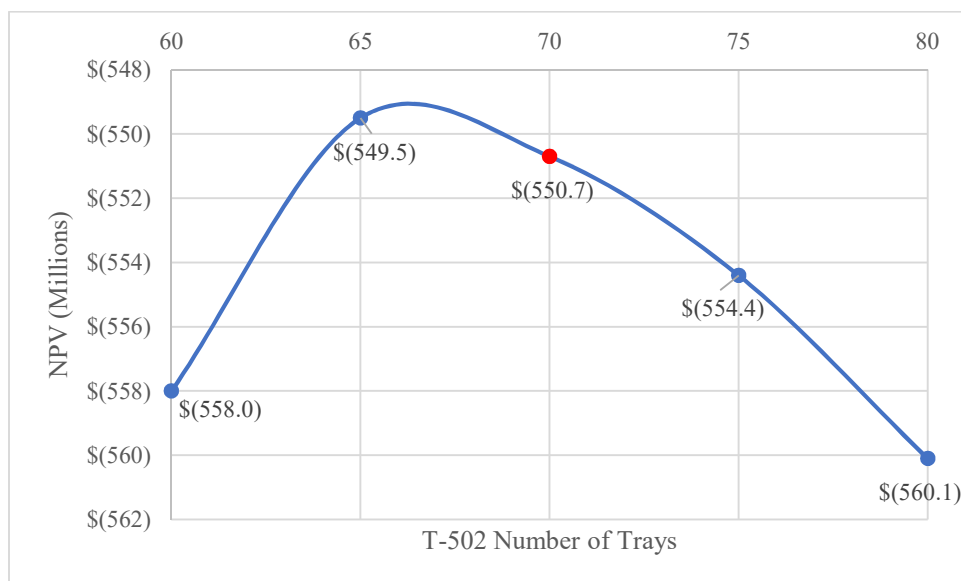


Figure 10: T-502 Number of Trays vs. Net Present Value

Next the top tray pressure was considered. As the top tray pressure increased, the temperature of the styrene product began to rise above 125°C at which styrene spontaneously polymerizes, but the net present value increased. The team decided that 27 kPa was the highest pressure in which the styrene product was kept low enough under this temperature. This gave a savings of about \$2 million.

The feed tray to T-502 was next considered. As stated above, the feed stream vapor/liquid fractions should match the feed tray vapor/liquid fractions to make the process the most economical. The feed tray of T-502 was changed from the base case tray of 25 to tray 30. The trays considered and their associated net present values are shown in **Error! Reference source not found..**

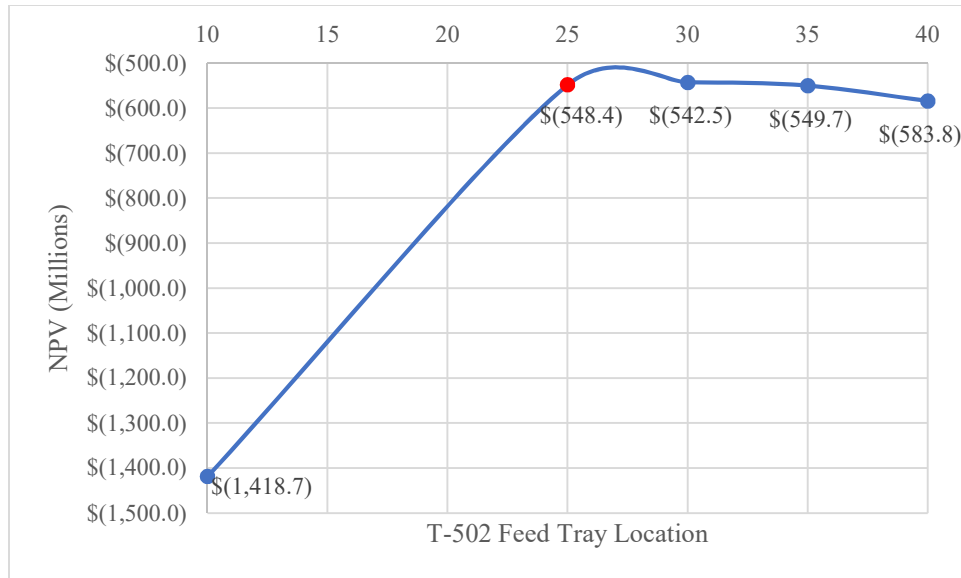


Figure 11: T-502 Feed Tray Location vs. Net Present Value

Compressor

A safety concern was recognized with the compressor due to the large compression ratio of 6:1 and the outlet temperature of the compressor. The compressor was split into two compressors each with a ratio of about 2.5:1. The adiabatic efficiency was updated from 60% to 80% to match literature values given in Table 11.10 of Turton (Turton 378-379). 80% was selected because rotary compressors are more adiabatically efficient than reciprocating compressors and heuristics provide 80% as the low end of the reciprocating compressor operating at a 3:1 compression ratio. This change in adiabatic efficiency reduced the outlet temperature of the compressors to 196°C which is within the maximum heuristics value of 204°C. The new arrangement of compressors is shown in *Figure 1*.

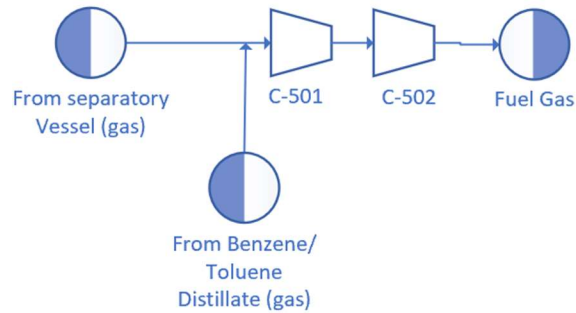


Figure 12: Updated Compressor PFD

This added compressor decreased the net present value by about \$300,000 and gave a final net present value of (\$543.4) million.

Heat Integration

Next, heat integration was completed. In the process, E-501 is the only heating heat exchanger and the only heat exchanger hot enough to heat the E-501 stream is E-503. Both exchangers use high pressure steam as their utility. The process streams of these two heat exchangers were crossed in E-501 and the new PFD is shown in *Figure* .

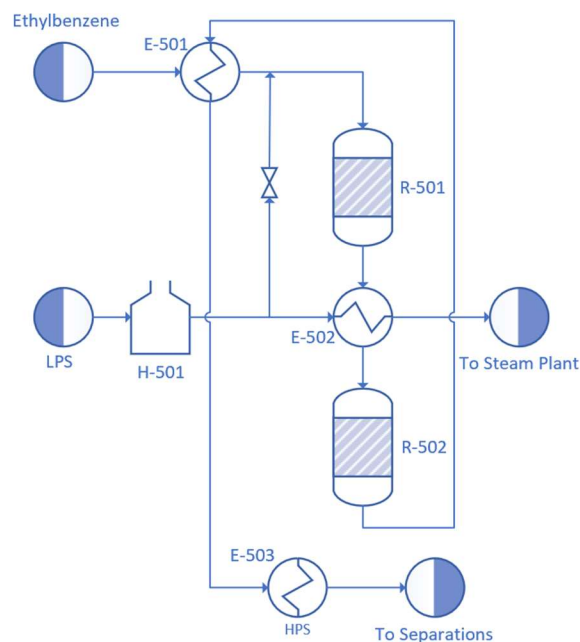


Figure 13: Heat Integrated PFD

Incorporating the heat integration provided about \$2 million savings and gave a net present value of (\$541.3) million.

Management Recommendations

After meeting with management, there were a couple of recommendations for improving the optimization as presented above. This section will outline those changes and their associated savings.

First, it was noted that a 5°C approach temperature is acceptable for refrigerated water. This allowed the inlet temperature of the three-phase separatory vessel to decrease to 10°C from 15°C. This provided a \$2.5 million savings due to further raw material and product recovery.

Next, it was recommended that a heat exchanger be added between the two compressors to decrease utility usage. After adding the intercooler, the net present value increased to the final optimized value of (\$532) million.

Overall, the team was able to increase the net present value by about \$390 million through the completion of one round of unit operation optimization and heat integration. The final optimized PFD can be found in Appendix B and the associated economic tables are found in Appendix C-E.

Process Safety

There are several aspects to process safety. These include but are not limited to environmental considerations, chemical safety, thermal issues surrounding pieces of equipment and proper training. Each issue is equally important and must be addressed to ensure that the proper measures are taken and put in place to establish a safe work environment for those who encounter the process.

Chemical Safety

To begin, chemical safety is one of the most obvious aspects when process safety in a chemical plant is considered. As mentioned previously, this particular process involves the dehydrogenation of ethylbenzene to create styrene. To do this, three reactions must take place, which means multiple chemicals are present. These chemicals include styrene, ethylbenzene, hydrogen, benzene, ethylene, toluene, and methane. While none of these chemicals pose a significant threat alone, together they may have the potential to cause major side effects. One way to determine the effect of a specific chemical is through software such as the Chemical Reactivity Worksheet. Through this one can see a chemical's effect on public health and how it may react when mixing with other chemicals. To increase process safety, these factors should be taken into consideration to determine the most efficient way to handle a situation in which a process was to malfunction.

Chemical Impact on Health

In the dehydrogenation process of ethylbenzene to produce styrene, the inhalation or concentration of vapors in air of the chemicals in the process contribute to the following side-effects:

Benzene: dizziness, nausea, vomiting, headache, coma

Ethylbenzene: blisters, irritation of nose, dizziness, irritation of eye

Ethylene: muscular weakness, dizziness, unconsciousness

Hydrogen: dizziness or asphyxiation without warning, irritations

Methane: high concentrations may cause asphyxiation

Styrene: moderate irritation; high concentrations can cause dizziness, drunkenness

Toluene: eye and upper respiratory irritation, irritation of skin

To combat some of these temporary side-effects, it is recommended that there be eye-washing equipment for chemical splashes as well as ventilation, flairs, and respiration for fumes at proper locations in the plant.

Aside from the “somewhat” temporary side effects of these chemicals mentioned above, some of these have the potential to cause long-term side effects and even contribute to death.

Benzene and styrene are labeled by the Department of Health and Human Services as carcinogens, or cancer-causing. Both can cause leukemia and lymphoma if there is long-term exposure to elevated levels of these chemicals.

No matter the effect on health, to protect against negative side effects, it is suggested that personal protective equipment (PPE) be worn. PPE includes protective eyewear, protective clothes, protective gloves, and earplugs to avoid any short or long-term side effects that come from contact with the process.

Reactions with other Chemicals

It has been determined that the majority of the chemicals within this process can mix without causing any hazardous reactivity. However, styrene and ethylene are both considered to be self-reactive. This is because both compounds can spontaneously polymerize at specific temperatures, and both are highly flammable.

To prevent these issues, it is recommended that there are gas detectors to swiftly detect when there is leakage of a gas and safety valves to help regulate pressure. Also, if possible, open ignition sources from the processing area should be removed. Lastly, equipment should be

grounded and bonded properly to prevent any static or electrical failure from becoming an ignition source.

Environmental Considerations

Less often considered are the effects of chemicals on the environment, if released into the atmosphere. Some chemicals within the process can not only contaminate the air in which it is released to, but could also attach to rain or snow and could be carried to the ground to contaminate water and soil. This may further contribute to the deaths of animals and plants in the area. Others can react with chemicals in the atmosphere to create smog. Hydrogen is particularly considered an indirect greenhouse gas due to its emissions leading to increased burdens of methane and ozone and thereby increasing global warming. Similarly, methane is also a greenhouse gas and furthermore is a hazardous pollutant that contributes to many premature deaths yearly.

For this process, it is recommended that the natural gas be sent to a flare system so that it may be burned and not harm the environment. It is also recommended that the piping be inspected often to ensure there are no cracks that can contribute to leaks. A detection system would also be effective to detect if any gas is leaking.

Thermal Issues

In the optimized process, streams are entering both reactors at temperatures above 500°C. This means that all streams surrounding this process, particularly in the pipes, are extremely hot. This makes this area a large safety hazard.

To manage this hazard, it is suggested that the pipes be in an isolated area that makes it difficult for workers to regularly encounter them. Also, these pipes should be labelled so that

those who do find themselves near these pipes will be cautious. Lastly, the pipes should be well insulated, that way the heat is not able to escape to the outside surface of the insulation in case someone were to come in contact with the insulation.

Training

Training serves as one of the most crucial factors in process safety. Training teaches the proper precautions and measures to take while in the processing plant. Therefore, it is recommended that those working in the plant have a great understanding of the specific chemical process taking place in the plant as well as the operating procedures. They should also fully understand the safety and emergency procedures in case a hazardous situation arises. It is also recommended that regular refresher training be conducted to ensure the highest degree of safety.

Recommendations/Considerations

It is recommended that the team continues with further project development. As previously mentioned, after one round of optimization, the net present value increased by roughly \$390 million from the base case net present value. The current market value of styrene that would be equivalent to the amount needed for this process is \$160 million per year. With one round of optimization, the cost to make styrene from this process is \$204 million. Through further optimization, it is anticipated that this value can decrease further and match the current market value of styrene. If this is completed, then making styrene will be considered more economically viable than purchasing it.

The next step in furthering project development would be the completion of a second round of unit operations optimization. The second round of optimization involves a process nearly identical to that of the first round of optimization. Through use of PRO/II, the team would

once again vary the variables within both reactors, the separatory vessel, and the columns, considering the effects that each change has on equipment downstream.

Following this, the team plans to implement some design optimization, specifically concerning the material of construction for the two distillation towers. Currently the towers are made of stainless steel clad. By changing these towers' materials to carbon steel, we expect about a \$4 million increase in the net present value.

Global Considerations

Taking into consideration the global climate, such as the global pandemic and international relations, there are supply chain upsets. Currently, the polystyrene plant has to rely on the market to purchase styrene for its process. Through the building of the styrene plant, the polystyrene plant will be less reliant on supply chain. Likewise, a reduction of international trade based on trade agreements could affect supply chain. Governing ideals at the time also have the potential to impact supply chain production.

PART 2: FLUIDIZED BED REACTOR

Introduction

Fluidized bed reactors (FBRs), often used in the petroleum and chemical processing industries, are a type of reactor known to be more efficient and advantageous over their counterparts. The reason for this popularity is due to their “superior heat transfer, ability to easily move solids like a fluid, and the ability to process materials with a wide particle size distribution” (Cocco 21). Fluidized bed reactors operate by passing a fluid through a solid material, typically a catalyst, at high speeds. This causes the solid to behave as a fluid, allowing for a more uniform process. Despite the advantages, these types of reactors do pose challenges such as being prone to erosion and higher operating costs.

The purpose of the tasked assignment was to design and optimize an isothermal fluidized bed reactor to convert ethylbenzene into styrene. This assignment serves as an extension of the Ch E 450 Styrene Case Study in which an adiabatic reactor was used, therefore, the same reactions and kinetics applied to this assignment. The optimization was completed through use of conditions given by management and a process design program, AVEVA PRO/II Simulation. The purpose was achieved through the changing of variables within the fluidized bed reactor and observing how changing these variables affected the reaction selectivity of styrene.

Designing the Process

To begin, the isothermal FBR had to be modeled in the simulation. Through the use of reactor and process design specifications provided by management, this was able to be achieved. In the process, the feed stream, stream 1, enters a splitter, in which 10% of this stream, stream 2,

acts as a bypass and enters a valve, which further passes through a heat exchanger before entering a mixer. The purpose of this heat exchanger is to regulate the temperature since adding the valve increased the stream temperature. The remaining 90% of the feed stream, stream 5, enters the isothermal fluidized bed reactor, exits and mixes with the bypass stream.

The next step was to determine what was happening in this designed process. In order to aid in better determining exactly what was occurring in the reactor, calculations were completed.

Below are calculations specific to the fluidized bed reactor:

$$(Eq. 1) \quad Re_{\rho, mf} = \frac{u_{mf} d_p \rho_g}{\mu_g} = [1135.69 + 0.0408 Ar]^{0.5} - 33.7$$

$$(Eq. 2) \quad Ar = \frac{d_p^3 (\rho_s - \rho_g) \rho_g g}{\mu_g^2}$$

where Eq. 1 is the particle Reynold's number calculated at the minimum fluidization velocity and Eq. 2 is Archimedes number. Explanations of terms may be found in the list of symbols on page ix of the document.

Other helpful calculations that could aid in determining what's taking place in the reactor are selectivity of styrene, conversion of ethylbenzene, L/D, length to diameter, ratio of the reactor, reactor volume, and pressure drop across the reactor bed.

Optimization Process

Following the process design, an optimizer was added in PRO/II to quickly and efficiently optimize the necessary variables specified by management. Optimizers function by performing multiple rounds of linear optimization until a maximum value of selectivity that meets all process requirements is reached, similar to the manual optimization method performed in Part 1 of the case study. Optimized variables included inlet feed pressure, inlet reactor temperature, reactor volume, and reactor L/D ratio.

Optimization Results

As previously mentioned, selectivity served as the determining factor in whether a variable was optimum. Selectivity is defined as the ratio of desired product formed to undesired product formed. In this process, styrene served as the desired product while benzene served as the undesired product. From the optimizer results, the highest selectivity of styrene in the reactor is 12.1. Optimum values for the variables mentioned may be found in the table below:

Table 1: Calculated Optimum Values

Variable	Optimum Value
Inlet Feed Pressure (bar)	3.9
Inlet Reactor Temperature (°C)	488.2
Reactor Volume (m ³)	196.2
Reactor L/D Ratio	2

Optimization Concerns

Although selectivity of styrene for this reactor is relatively high, other calculations allow for the full scope of the process to be seen. In particular, the conversion of ethylbenzene in the process is .0500. This conversion is quite low and can have a major impact on the complete ethylbenzene to styrene process by increasing the recycle stream, as was previously seen in the Ch E 450 Styrene Case Study. This low conversion can also impact downstream equipment, making it so that equipment must increase drastically in size, ultimately negatively impacting the net present value of the plant. As a result, from this simulation alone, it cannot be determined whether the original adiabatic reactor or the newly optimized fluidized bed reactor is more economically feasible and practical for the process at hand. To determine this, the entire process,

including the fluidized bed reactor, needs to be simulated and optimized similar to the adiabatic reactor in the case study.

Conclusion

In conclusion, having a high selectivity does not guarantee that the process is always feasible. Other factors play a large role in determining the reasonableness of a process. In some ways, what may be initially considered “optimum” based on a single objective function may actually not be the best option for the process and instead a value that is either greater or lower may be what best suits the process.

LIST OF REFERENCES

Cocco, Ray & Karri, Sb & Knowlton, Ted. (2014). Introduction to Fluidization. Chemical Engineering Progress. 110. 21-29.

Turton, Richard. *Analysis, Synthesis, and Design of Chemical Processes*. Fifth Edition. Upper Saddle River: Prentice Hall, 2018.

Appendix A: Base Case Process Flow Diagram



Appendix B: Optimized Process Flow Diagram

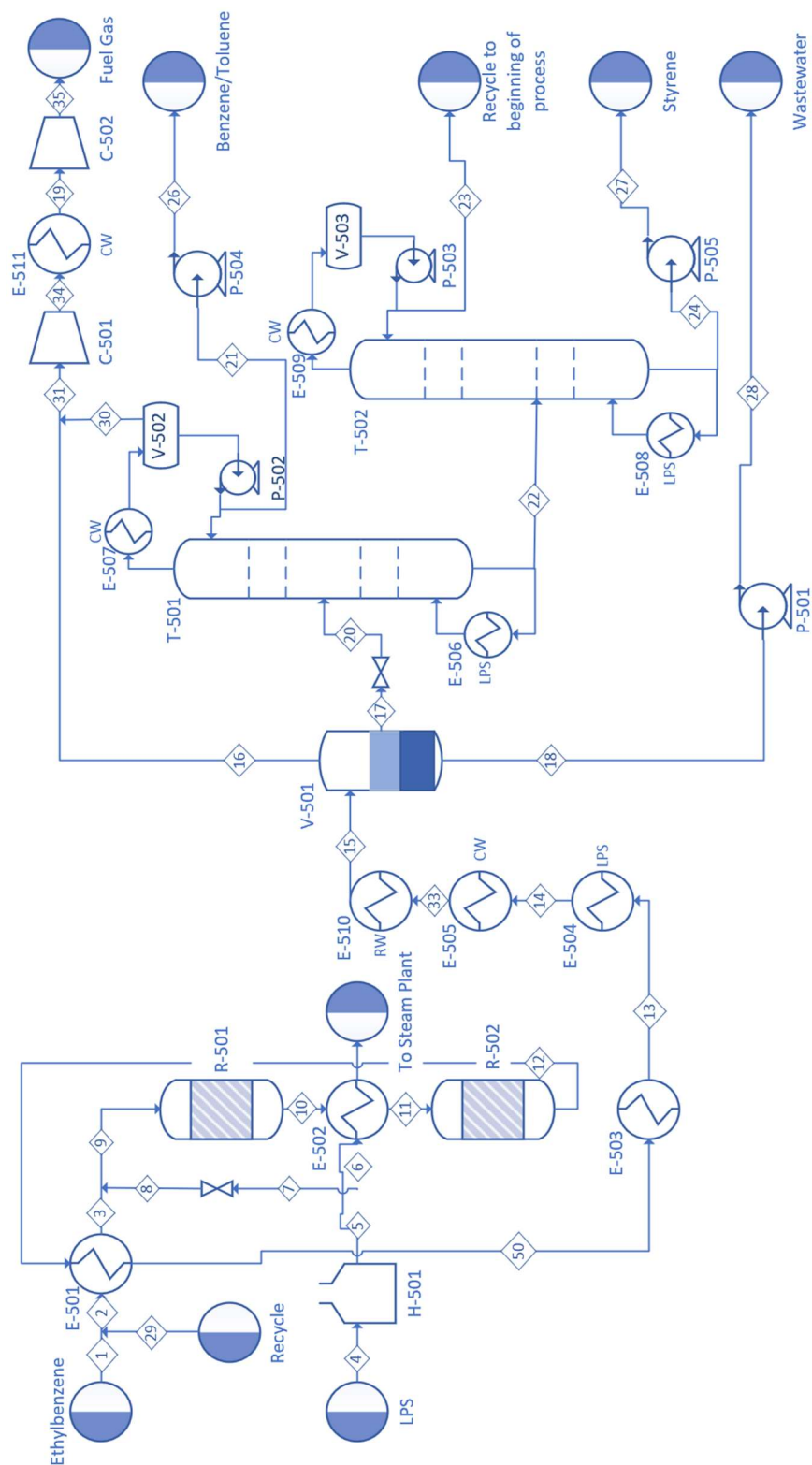


Figure 13: Optimized Process Flow Diagram

Appendix C: Optimized Stream Table (See Excel Appendix)

Table 2: Optimized Stream Table

Stream No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Temperature (°C)	136	108	225	159	879	879	879	878	550	522	562	546	270	180	10
Pressure (kPa)	235	235	215	600	565	565	565	215	215	204	189	176	161	146	116
Vapor Mole Fraction	0	0	1	1	1	1	1	1	1	1	1	1	1	1	0.030834
Total Flow (kg/h)	20,261	68,359	68,359	147,725	102,547	32,288	70,260	70,260	138,619	138,619	138,619	138,619	138,624	138,624	138,624
Total Flow (kmol/h)	191.6	644.7	644.7	8200.0	5692.2	1792.2	3900.0	3900.0	4544.7	4630.2	4630.2	4690.1	4690.1	4690.1	4690.1
Component Flows															
Water	0.0	0.0	0.0	8200.0	5692.2	1792.2	3900.0	3900.0	3900.0	3900.0	3900.0	3900.0	3900.0	3900.0	3900.0
Ethylbenzene	187.8	639.3	639.3	0.0	0.0	0.0	0.0	0.0	639.3	540.5	540.5	456.8	456.8	456.8	456.8
Styrene	0.0	1.2	1.2	0.0	0.0	0.0	0.0	0.0	1.2	76.3	76.3	121.3	121.3	121.3	121.3
Hydrogen	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	61.8	61.8	82.9	82.9	82.9	82.9
Benzene	1.9	1.9	1.9	0.0	0.0	0.0	0.0	0.0	1.9	12.4	12.4	27.2	27.2	27.2	27.2
Toluene	1.9	2.3	2.3	0.0	0.0	0.0	0.0	0.0	2.3	15.5	15.5	39.5	39.5	39.5	39.5
Ethylene	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	10.5	10.5	25.2	25.2	25.2	25.2
Methane	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	13.2	13.2	37.2	37.2	37.2	37.2

16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33
10	10	10	40	10	50	125	93	125	700	50	122	10	95	50	14	10	40
116	116	116	98	60	50	70	27	57	550	200	200	200	235	50	50	50	131
1	0	0	1	0.000516	0	0	0	0	1	0	0	0	0	1	1	1	0.033346
1,515	66,922	70,186	1,932	66,922	5,882	60,624	48,098	12,525	32,288	5,882	12,525	70,186	48,098	417	1,932	0	0
144.6	649.8	3895.7	153.5	649.8	67.5	573.4	453.1	120.3	1792.2	67.5	120.3	3895.7	453.1	8.9	153.5	144.6	4690.1
1.5	2.8	3895.6	3.7	2.8	0.7	0.0	0.0	0.0	1792.2	0.7	0.0	3895.6	0.0	2.2	3.7	1.5	3900.0
0.5	456.3	0.0	0.5	456.3	4.5	451.7	451.5	0.2	0.0	4.5	0.2	0.0	451.5	0.1	0.5	0.5	456.8
0.1	121.2	0.0	0.1	121.2	0.0	121.2	1.2	120.0	0.0	0.0	120.0	0.0	1.2	0.0	0.1	0.1	121.3
82.8	0.1	0.0	82.9	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	82.9	82.8	82.9
0.3	26.8	0.0	2.7	26.8	24.5	0.0	0.0	0.0	0.0	24.5	0.0	0.0	0.0	2.3	2.7	0.3	27.2
0.1	39.3	0.0	1.4	39.3	37.7	0.4	0.4	0.0	0.0	37.7	0.0	0.0	0.4	1.2	1.4	0.1	39.5
22.9	2.3	0.0	25.2	2.3	0.1	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	2.3	25.2	22.9	25.2
36.4	0.8	0.1	37.1	0.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.8	37.1	36.4	37.2

34	35	50
127	75	429
240	98	176
1	1	1
0	0	0
153.5	153.5	4690.1
3.7	3.7	3900.0
0.5	0.5	456.8
0.1	0.1	121.3
82.9	82.9	82.9
2.7	2.7	27.2
1.4	1.4	39.5
25.2	25.2	25.2
37.1	37.1	37.2

Appendix D: Utility Table (See Excel Appendix)

Table 3: Utility Table

Exchanger	E-501	E-502	E-503	E-504	E-505	E-510	E-506	E-507	E-508	E-509	E-511
In			bftw	bftw	CW	RW	lps	CW	lps	CW	CW
Out			hps	lps	30	5	bftw	30	bftw	30	30
Temp (°C)		878.5	115	115					160		
Pressure (Bar)		4.64	0.69	0.69	1.01	1.01	5.00	1.01	5.00	1.01	1.01
Rate (kg/h)		32287.6	10000.0	100000.0	3663615.9	318301.6	16022.5	470218.8	61138.0	2089312.3	3119.9
Rate (MT/h)		32.3	10.0	100.0	3663.6	318.3	16.0	470.2	61.1	2089.3	3.1
Rate (MJ/hr)		13501.6	47605.1	24483.6	228394.5	13386.8	33357.3	19563.9	127283.3	130250.4	194.5
Rate (GJ/hr)		13.5016	47.6051	24.4836	228.3945	13.3868	33.3573	19.5639	127.2833	130.2504	0.1945

Appendix D.2: Equipment Summary (See Excel Appendix)

Table 4: Equipment Summary

Equipment Pricing Summary														CEPCI		2001	2016	Inflation		2023	622.2						
		Equipment Size (A)		Equip Qty			C ⁰ (2001.00)		F _p	F _p ⁰	F _M	F _M ⁰	F _q	F _q ⁰	F _{BM}	F _{BM} ⁰											
Tag	Description	Tot Required	Purch ea	Base	Spares	Total	Each	Total	F _p	F _p ⁰	F _M	F _M ⁰	F _q	F _q ⁰	F _{BM}	F _{BM} ⁰	2001	2023	2001	2023							
Heat exchangers																											
E-501	Fixed TS	410.5	410.5	1	0	1	44,543	44,543	0.99	1.00	1.00	1.00	N/A	3.281	3.290		146,546	229,691	146,139	229,053							
E-502	Flt Head	258.9	258.9	1	0	1	42,969	42,969	1.00	1.00	2.70	1.00	N/A	6.114	3.290		141,369	221,577	262,708	411,759							
E-503	Fixed TS	1,346.3	673.1	2	0	2	59,523	119,045	1.05	1.00	2.70	1.00	N/A	6.341	3.290		391,658	613,870	754,913	1,183,222							
E-504	Fixed TS	1,187.7	593.8	2	0	2	55,126	110,252	1.00	1.00	1.00	1.00	N/A	3.292	3.290		362,730	568,530	362,924	568,834							
E-505	Fixed TS	2,891.4	963.8	3	0	3	75,074	225,223	1.00	1.00	1.00	1.00	N/A	3.290	3.290		740,982	1,161,388	740,982	1,161,388							
E-506	Kettle Reboiler	294.2	294.2	3	0	3	95,989	287,967	1.00	1.00	1.00	1.00	N/A	3.292	3.290		947,412	1,484,938	948,023	1,485,969							
E-507	Flt Head	627.8	627.8	1	0	1	88,036	88,036	1.00	1.00	1.00	1.00	N/A	3.290	3.290		289,639	453,969	289,639	453,969							
E-508	Kettle Reboiler	1,122.4	1,122.4	12	0	12	91,398	1,096,770	1.00	1.00	1.00	1.00	N/A	3.292	3.290		3,608,373	5,655,630	3,610,703	5,659,282							
E-509	Flt Head	1,139.6	1,139.6	2	0	2	80,529	161,058	1.00	1.00	1.00	1.00	N/A	3.290	3.290		529,880	830,514	529,880	830,514							
E-510																	162,948	255,398	162,948	255,398							
E-511																	51,342	80,471	51,342	80,471							
Pumps & Drives																											
P-501 A/B	Centrifugal	1.63	1.63	1	1	2	2,556	5,112	1.00	1.00	1.60	1.00	N/A	4.05	3.24		16,564	25,962	20,705	32,453							
P-504 A/B	Centrifugal	0.29	1.00	1	1	2	2,450	4,900	1.00	1.00	1.60	1.00	N/A	4.05	3.24		15,877	24,885	19,847	31,107							
P-505 A/B	Centrifugal	0.61	1.00	1	1	2	2,450	4,900	1.00	1.00	1.60	1.00	N/A	4.05	3.24		15,877	24,885	19,847	31,107							
P-506 A/B	Centrifugal	3.44	3.44	1	1	2	2,898	5,797	1.00	1.00	1.60	1.00	N/A	4.05	3.24		18,782	29,439	23,478	36,798							
Drives																											
PD-501 A/B	Elec Exp Proof	3.27	3.27	1	1	2	1,388	2,776	N/A	N/A	N/A	N/A	N/A	1.500	1.500		4,164	6,526	4,164	6,526							
PD-504 A/B	Elec Exp Proof	0.58	1.00	1	1	2	289	577	N/A	N/A	N/A	N/A	N/A	1.500	1.500		866	1,357	866	1,357							
PD-505 A/B	Elec Exp Proof	1.11	1.11	1	1	2	334	668	N/A	N/A	N/A	N/A	N/A	1.500	1.500		1,002	1,570	1,002	1,570							
PD-506 A/B	Elec Exp Proof	8.59	8.59	1	1	2	4,258	8,516	N/A	N/A	N/A	N/A	N/A	1.500	1.500		12,774	20,021	12,774	20,021							
Heater(s)																											
H-501	Fired Non-Rx	77,121.4	77,121.4	1	0	1	3,098,803	3,098,803	1.000	1.000	1	1	N/A	2.800	2.100		6,507,486	10,199,592	8,676,648	13,599,456							
Reactor(s)																											
R-501	Pkd Bed	277.1	55.4	5	0	5	40,368	201,838	1.00	1.00	3.10	1.00	N/A	7.892	4.07		821,479	1,287,556	1,592,903	2,496,656							
R-502	Pkd Bed	277.1	55.4	5	0	5	40,368	201,838	1.00	1.00	3.10	1.00	N/A	7.892	4.07		821,479	1,287,556	1,592,903	2,496,656							
Vessels																											
V-501	Vertical	24.4	24.4	1	0	1	21,219	21,219	1.00	1.00	1.00	1.00	N/A	4.07	4.07		86,363	135,362	86,363	135,362							
V-502	Horizontal	7.5	7.5	1	0	1	9,034	9,034	1.00	1.00	1.00	1.00	N/A	3.01	3.01		27,191	42,619	27,191	42,619							
V-503	Horizontal	64.7	64.7	1	0	1	34,433	34,433	1.00	1.00	1.00	1.00	N/A	3.39	3.01		103,644	162,448	116,729	182,956							
Vessel Internals N/A																											
Towers																											
T-501	Distillation Column	397.80	397.80	1	0	1	245,011	245,011	1.00	1.00	1.75	1.00	N/A	5.435	4.07		997,195	1,562,967	1,331,636	2,087,156							
T-502	Distillation Column	4217.58	468.62	9	0	9	289,320	2,603,877	1.00	1.00	1.75	1.00	N/A	5.435	4.07		10,597,779	16,610,564	14,152,070	22,181,429							
Tower Internals																											
TI-501	Sieve Trays	13.28	1.08	100	0	100	1,024	102,385	N/A	N/A	N/A	N/A	1	1.8	1		102,385	160,475	184,293	288,855							
C-502	Sieve Trays	76.34	6.21	672	0	672	3,962	2,662,220	N/A	N/A	N/A	N/A	1	1.8	1		2,662,220	4,172,664	4,791,996	7,510,796							
Compressors & Drives																											
EDS7																											
C-501	Rotary	92.80	92.80	1	0	1	48,801	48,801	N/A	N/A	N/A	N/A	N/A	2.4	2.4		117,122	183,573	117,122	183,573							
CD-501	Electrical/ Exp Proof	92.80	92.80	1	0	1	36,015	36,015	N/A	N/A	N/A	N/A	N/A	1.5	1.5		54,022	84,673	54,022	84,673							
C-502	Rotary	137.93	137.93	1	0	1	91,627	91,627	N/A	N/A	N/A	N/A	N/A	2.4	2.4		219,905	222,322	219,905	222,322							
CD-502	Electrical/ Exp Proof	137.93	137.93	1	0	1	47,167	47,167	N/A	N/A	N/A	N/A	N/A	1.5	1.5		70,751	71,529	70,751	71,529							
Total								11,485,539	Total								Rounded Up		(30,648,000)	(47,875,000)	(40,978,000)	(64,065,000)					
Total Module (CTM)																CTM						\$ (48,353,348.82) \$ (75,596,420.02)					
Grass Roots																Rounded Up						\$ - \$ -					
																CGR						\$ (63,677,252.56)		\$ (99,533,680.76)			
																CGR/FCI Round						\$ (63,678,000.00)		\$ (99,534,000.00)			
																Bldg											
Land																											
Total Investment																											
start value																											

Appendix E: Income Cash Flow Statement (See Excel Appendix)

Table 5: Income Cash Flow Statement

Income and Cash Flow Statement															
End of Year	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032	2033	2034	2035
Income Statement															
Revenue	209,001,518.98	209,001,518.98	209,001,518.98	209,001,518.98	209,001,518.98	209,001,518.98	209,001,518.98	209,001,518.98	209,001,518.98	209,001,518.98	209,001,518.98	209,001,518.98	209,001,518.98	209,001,518.98	209,001,518.98
Expenses	186,608,499.09	186,614,731.33	186,614,731.33	186,614,731.33	186,614,731.33	186,614,731.33	186,614,731.33	186,614,731.33	186,614,731.33	186,614,731.33	186,614,731.33	186,614,731.33	186,614,731.33	186,614,731.33	186,614,731.33
Materials	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Catalyst	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Labor	3%	3%	3%	3%	3%	3%	3%	3%	3%	3%	3%	3%	3%	3%	3%
Utilities (Cur)	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Waste Treatment (Cwr)	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Other (Ccr) = 0.18*F(Cr+1.73*Cr + 0.23*Cr)+Ccr+Cwr															
Conv-HO (0.18*F(Cr))															
Conv-HW (0.23*F(Cwr))															
Conv-Cr (1.73*F(Cr))															
Conv-HW (0.23*F(Cwr))															
Depreciation															
Land															
Land (BV)															
Building															
Bldg BV															
Machines															
Mach BV															
Net Income															
Income Taxes															
PV @ 5/U															
Cash Flow Statement															
Operating Activities															
Net Income															
Depreciation															
Investment Activities															
Land															
Purchase															
Sale															
Book Value															
Taxes															
Net Gain/(Loss)															
Net Cash Flow															
PV @ 5/U															
Buildings															
Purchase															
Sale															
MACRS factor															
Depreciation															
Book Value															
Taxes															
Net Gain/(Loss)															
Net Cash Flow															
PV @ 5/U															
Machines (FCI or Cost ex buildings and land)															
Purchase															
Sale															
Depreciation															
Book Value															
Taxes															
Net Gain/(Loss)															
Net Cash Flow															
PV @ 5/U															
Financing Activities															
Working Capital															
Cur 3 months															
NPV															
Cur 6 months															
NPV															
Net Cash Flow															
Cumulative Cash Flow															
PV @ 5/U @ (12.0%)															
Cumulative Discounted CF															
Summary Project Metrics															
MARR	12%														
DCR/IRR	12.0%														

